2-Fluorobenzoic acid, phenyl ester

Inchi: InChI=1S/C13H9FO2/c14-12-9-5-4-8-11(12)13(15)16-10-6-2-1-3-7-10/h1-9H
InchiKey: PJKSIUSOWPXUMO-UHFFFAOYSA-N
Formula: C13H9FO2
SMILES: O=C(Oc1ccccc1)c1ccccc1F
Mol. weight [g/mol]: 216.21

Physical Properties

Property code	Value	Unit	Source
gf	-154.96	kJ/mol	Joback Method
hf	-290.97	kJ/mol	Joback Method
hfus	22.99	kJ/mol	Joback Method
hvap	58.09	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.045		Crippen Method
mcvol	155.720	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1642.00		NIST Webbook
rinpol	1642.00		NIST Webbook
tb	630.74	K	Joback Method
tc	867.75	K	Joback Method
tf	374.38	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.72	J/mol×K	630.74	Joback Method
cpg	387.46	J/mol×K	670.24	Joback Method
cpg	400.13	J/mol×K	709.74	Joback Method
cpg	411.78	J/mol×K	749.25	Joback Method
cpg	422.45	J/mol×K	788.75	Joback Method
cpg	432.17	J/mol×K	828.25	Joback Method
cpg	441.00	J/mol×K	867.75	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume